Supporting Information for Conformational Preferences of 3-(Dimethylazinoyl)propanoic Acid as a Function of pH and Solvent; Intermolecular vs. Intramolecular Hydrogen Bonding

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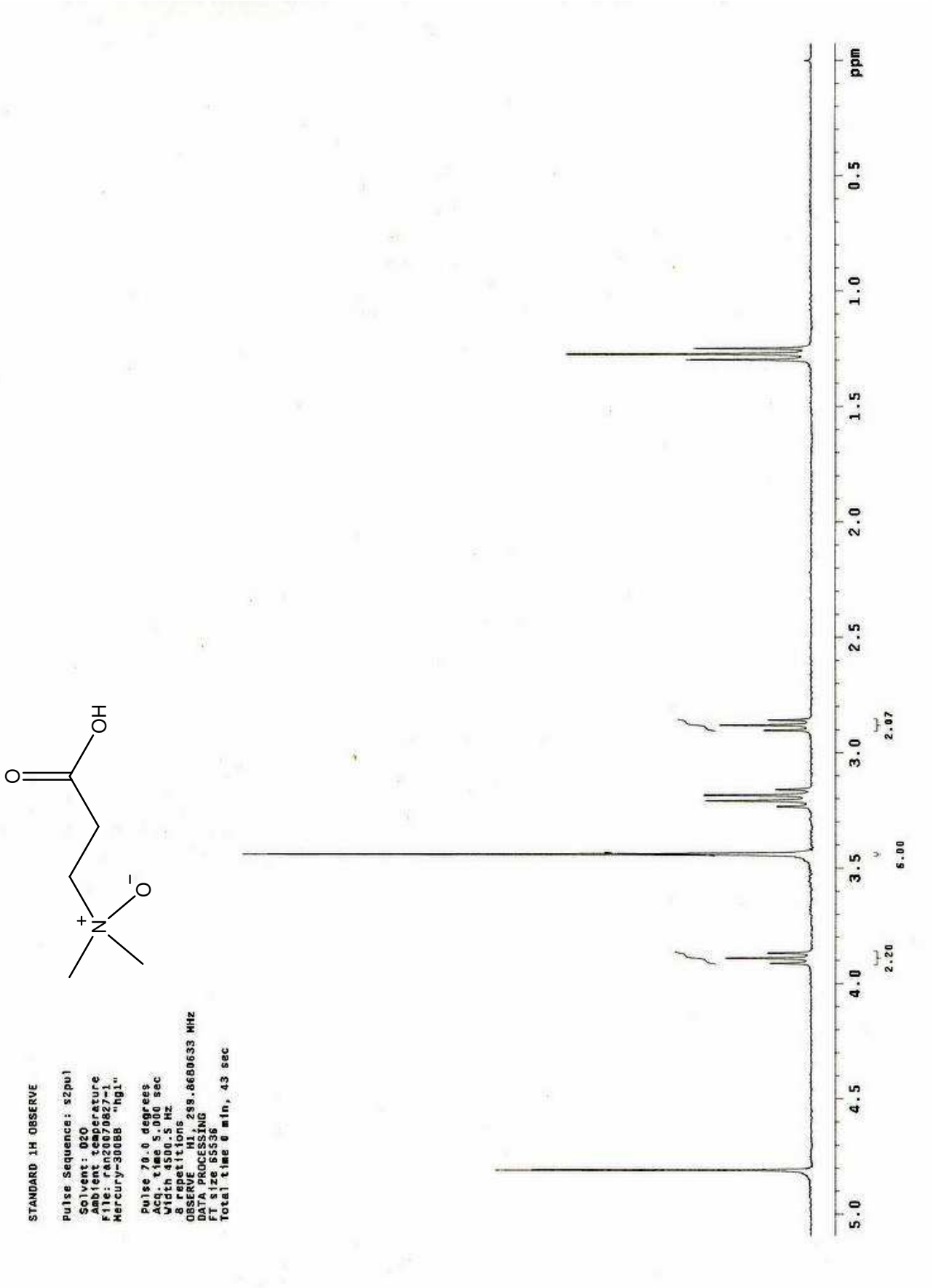
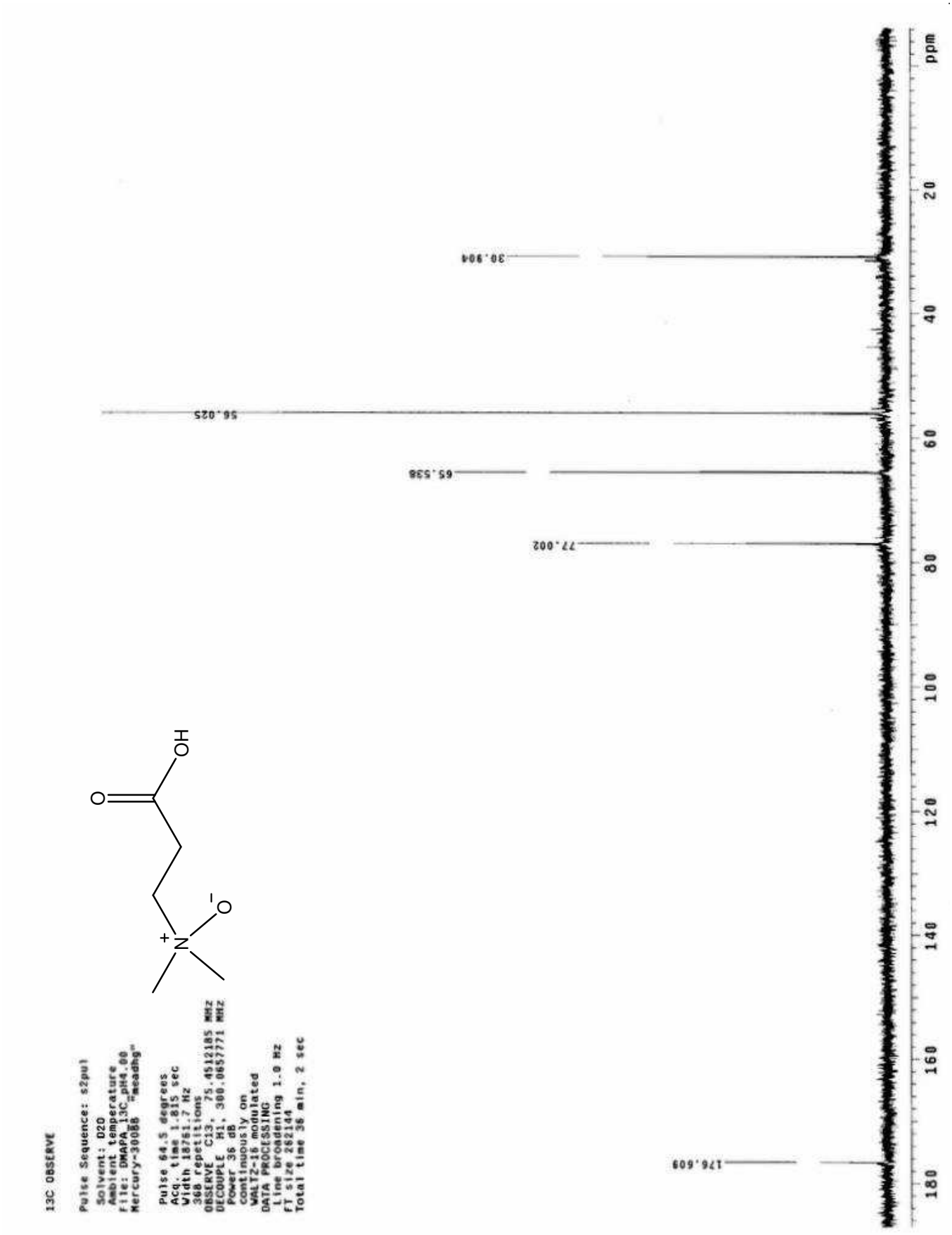
Table of Contents

^{1}H NMR of 3-(Dimethylazinoyl)propanoic acid



^{13}C NMR of 3-(Dimethylazinoyl)propanoic acid



Computational Data

Extracted coupling constants for DMAPA with pH

	$^3J_{obs}$, Hz			$^3J_{obs}$, Hz			$^3J_{obs}$, Hz	
pH	J_{13}	J_{14}	pH	J_{13}	J_{14}	pH	J_{13}	J_{14}
0.3	7.2	7.2	3.8	6.7	6.7	6.8	6.4	8.9
0.5	7.0	7.0	4.0	6.6	6.7	7.2	6.3	9.0
1.1	7.0	7.0	4.3	6.7	6.8	7.7	6.3	9.1
1.3	6.9	6.9	4.4	6.7	6.8	7.9	6.3	9.1
1.8	6.9	6.9	4.8	6.8	6.9	8.1	6.3	9.1
2.5	6.9	6.9	5.1	6.7	7.2	8.2	6.4	9.1
2.6	6.8	6.8	5.2	6.6	7.4	8.3	6.3	9.1
2.9	6.8	6.8	5.6	6.6	8.1	8.7	6.4	9.2
3.1	6.8	6.8	6.4	6.5	8.7	9.4	6.4	9.2
3.6	6.7	6.7	6.7	6.5	8.7	9.7	6.3	9.2
						9.9	6.2	9.2

Cartesian Coordinates and Total Energy Data

3-(dimethylazinoyl)propanoic acid (protonated gauche)

```
Distributed Data Interface kickoff program.
 Initiating 1 compute processes on 1 nodes to run the following command:
 C:\WinGAMESS/gamess.06.exe protonated-gauche01

          ***************************************************
          *          GAMESS VERSION =  7 SEP 2006 (R4)          *
          *              FROM IOWA STATE UNIVERSITY             *
          * M.W.SCHMIDT, K.K.BALDRIDGE, J.A.BOATZ, S.T.ELBERT, *
          *   M.S.GORDON, J.H.JENSEN, S.KOSEKI, N.MATSUNAGA,   *
          *           K.A.NGUYEN, S.J.SU, T.L.WINDUS,          *
          *        TOGETHER WITH M.DUPUIS, J.A.MONTGOMERY      *
          *          J.COMPUT.CHEM.  14, 1347-1363(1993)       *
          ******************** PC-UNIX VERSION ******************

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     MIE UNIVERSITY: HIROAKI UMEDA
     MICHIGAN STATE UNIVERSITY:
          KAROL KOWALSKI, MARTA WLOCH, PIOTR PIECUCH
     UNIVERSITY OF SILESIA: MONIKA MUSIAL, STANISLAW KUCHARSKI
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     INSTITUTE FOR MOLECULAR SCIENCE: KAZUYA ISHIMURA AND SHIGERU NAGASE
     UNIVERSITY OF NOTRE DAME: DAN CHIPMAN
     KYUSHU UNIVERSITY:
          FENG LONG GU, JACEK KORCHOWIEC, MARCIN MAKOWSKI, AND YURIKO AOKI
     PENNSYLVANIA STATE UNIVERSITY:
          TZVETELIN IORDANOV, CHET SWALINA, SHARON HAMMES-SCHIFFER

 EXECUTION OF GAMESS BEGUN Wed Oct 10 20:52:24 2007
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           ECHO OF THE FIRST FEW INPUT CARDS -
INPUT CARD> $CONTRL RUNTYP=OPTIMIZE $END
INPUT CARD> $DFT DFTTYP=B3LYP $END
INPUT CARD> $BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.T. $END
INPUT CARD> $CONTRL ICHARG=1 $END
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INPUT CARD>N        7.0        0.863259       -0.090267       -0.218695
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INPUT CARD>H        1.0        0.416824        1.609563        0.964933
INPUT CARD>H        1.0       -0.210125        1.686383       -0.698664
INPUT CARD>H        1.0       -2.025817        1.462945        0.905472
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                                 ----------------------
                                 GRADIENT (HARTREE/BOHR)
                                 ----------------------
       ATOM     ZNUC       DE/DX         DE/DY         DE/DZ
------------------------------------------------------------
 1  C            6.0    -0.0000224     0.0000366     0.0000160
 2  C            6.0     0.0000003    -0.0000108    -0.0000211
 3  C            6.0    -0.0000647    -0.0000333     0.0000081
 4  N            7.0     0.0000715     0.0000296     0.0000692
 5  C            6.0     0.0000256     0.0000157    -0.0000197
 6  C            6.0     0.0000291    -0.0000145    -0.0000264
 7  O            8.0     0.0000169    -0.0000944    -0.0000269
 8  O            8.0     0.0000668    -0.0000044    -0.0000532
 9  O            8.0    -0.0000229     0.0000097     0.0000526
10  H            1.0    -0.0000243     0.0000004     0.0000022
11  H            1.0    -0.0000105     0.0000074     0.0000015
12  H            1.0     0.0000039    -0.0000081     0.0000056
13  H            1.0    -0.0000083     0.0000185     0.0000093
14  H            1.0    -0.0000121     0.0000260     0.0000065
15  H            1.0    -0.0000150    -0.0000092    -0.0000298
16  H            1.0     0.0000067    -0.0000361     0.0000389
```

```
17  H           1.0    -0.0000010     0.0000130    -0.0000048
18  H           1.0     0.0000144     0.0000080    -0.0000156
19  H           1.0    -0.0000017    -0.0000072     0.0000087
20  H           1.0     0.0000080     0.0000262    -0.0000003
21  H           1.0    -0.0000603     0.0000268    -0.0000209

         MAXIMUM GRADIENT =  0.0000944    RMS GRADIENT = 0.0000296

     ***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF ALL ATOMS ARE (ANGS)
  ATOM   CHARGE       X              Y              Z
------------------------------------------------------------
C           6.0  -0.1063984842   1.0053394556   0.1468374829
C           6.0  -1.4543446099   0.5052559229   0.6742959531
C           6.0  -2.3070870390  -0.2997916698  -0.2871043447
N           7.0   0.9572385327  -0.0331659069  -0.2185974808
C           6.0   2.2807647182   0.6652567723  -0.3954761391
C           6.0   1.0875221570  -1.1468785133   0.7849716105
O           8.0   0.7024874992  -0.5921044981  -1.4989455394
O           8.0  -3.5881371935  -0.2835709126   0.0490101327
O           8.0  -1.8726693760  -0.9251217213  -1.2477556566
H           1.0   0.3505664390   1.6300059773   0.9181574716
H           1.0  -0.2244979127   1.6035138628  -0.7591110455
H           1.0  -2.0209985127   1.3955135451   0.9698501180
H           1.0  -1.3478226340  -0.0802012630   1.5954712495
H           1.0   2.9771564524  -0.0611907801  -0.8117372904
H           1.0   2.6240025522   1.0269915633   0.5746975187
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H           1.0   0.1700488626  -1.7335653816   0.7852836686
H           1.0   1.2806823244  -0.7160571101   1.7691690198
H           1.0  -4.1021071653  -0.8402288990  -0.5663373607
H           1.0  -0.2772636988  -0.8185188368  -1.5090792577

          TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS
      ATOM          MULL.POP.    CHARGE          LOW.POP.     CHARGE
   1 C              6.110618   -0.110618         6.186044   -0.186044
   2 C              6.460229   -0.460229         6.269730   -0.269730
   3 C              5.456408    0.543592         5.753101    0.246899
   4 N              7.449870   -0.449870         7.119116   -0.119116
   5 C              6.195542   -0.195542         6.260792   -0.260792
   6 C              6.255326   -0.255326         6.266820   -0.266820
   7 O              8.183080   -0.183080         8.335405   -0.335405
   8 O              8.391076   -0.391076         8.282604   -0.282604
   9 O              8.481093   -0.481093         8.356283   -0.356283
  10 H              0.795744    0.204256         0.784246    0.215754
  11 H              0.778359    0.221641         0.772808    0.227192
  12 H              0.774179    0.225821         0.774989    0.225011
  13 H              0.781639    0.218361         0.781405    0.218595
  14 H              0.774499    0.225501         0.780276    0.219724
  15 H              0.796825    0.203175         0.797027    0.202973
  16 H              0.786217    0.213783         0.784993    0.215007
  17 H              0.781260    0.218740         0.781473    0.218527
  18 H              0.794080    0.205920         0.786770    0.213230
  19 H              0.794395    0.205605         0.792510    0.207490
  20 H              0.599494    0.400506         0.661463    0.338537
  21 H              0.560070    0.439930         0.672144    0.327856
```

```
        ------------------------------
        BOND ORDER AND VALENCE ANALYSIS     BOND ORDER THRESHOLD=0.050
        ------------------------------

                    BOND                          BOND                          BOND
 ATOM PAIR DIST   ORDER       ATOM PAIR DIST   ORDER       ATOM PAIR DIST   ORDER
   1   2  1.531  1.042         1   3  2.595 -0.068         1   4  1.531  0.749
   1   5  2.471 -0.071         1   6  2.543 -0.067         1   7  2.432  0.113
   1  10  1.093  0.907         1  11  1.092  0.934         2   3  1.516  1.005
   2   6  3.034  0.051         2   8  2.359 -0.056         2   9  2.432 -0.057
   2  12  1.096  0.896         2  13  1.097  0.930         3   8  1.325  1.153
   3   9  1.226  1.734         4   5  1.507  0.831         4   6  1.505  0.866
   4   7  1.420  1.397         4   9  3.141  0.122         5   6  2.470 -0.065
   5   7  2.300 -0.091         5  14  1.089  0.943         5  15  1.091  0.936
   5  16  1.089  0.940         6  17  1.089  0.948         6  18  1.089  0.930
   6  19  1.092  0.929         7  21  1.006  0.636         8  20  0.976  0.779
   9  21  1.620  0.146

                      TOTAL       BONDED        FREE
     ATOM            VALENCE     VALENCE     VALENCE
   1 C                 3.520       3.520       0.000
   2 C                 3.856       3.856       0.000
   3 C                 3.792       3.792       0.000
   4 N                 4.055       4.055       0.000
   5 C                 3.416       3.416       0.000
   6 C                 3.533       3.533       0.000
   7 O                 1.955       1.955       0.000
   8 O                 1.872       1.872       0.000
   9 O                 1.959       1.959       0.000
  10 H                 0.925       0.925       0.000
  11 H                 0.923       0.923       0.000
  12 H                 0.924       0.924       0.000
  13 H                 0.923       0.923       0.000
  14 H                 0.926       0.926       0.000
  15 H                 0.928       0.928       0.000
  16 H                 0.930       0.930       0.000
  17 H                 0.929       0.929       0.000
  18 H                 0.934       0.934       0.000
  19 H                 0.927       0.927       0.000
  20 H                 0.835       0.835       0.000
  21 H                 0.826       0.826       0.000

        ---------------------
        ELECTROSTATIC MOMENTS
        ---------------------

POINT   1           X           Y           Z (BOHR)    CHARGE
              -0.918706   -0.273276   -0.461890        1.00 (A.U.)
        DX          DY          DZ         /D/  (DEBYE)
    2.440476    1.696228    3.410396    4.523706
...... END OF PROPERTY EVALUATION ......
STEP CPU TIME =     2.97 TOTAL CPU TIME =    41537.0 (  692.3 MIN)
TOTAL WALL CLOCK TIME=   100012.4 SECONDS, CPU UTILIZATION IS  41.53%
 $VIB
         IVIB=   0 IATOM=   0 ICOORD=   0 E=     -477.6763595412
-2.242882807E-05 3.657873066E-05 1.601658343E-05 2.837344957E-07-1.076149714E-05
-2.107507482E-05-6.471547112E-05-3.333946497E-05 8.076244982E-06 7.152259903E-05
 2.962861054E-05 6.921444492E-05 2.557738957E-05 1.569717202E-05-1.972253752E-05
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 2.908475478E-05-1.450618559E-05-2.643717104E-05 1.692908925E-05-9.442165883E-05
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 9.692749708E-06 5.264778681E-05-2.427922208E-05 4.315306908E-07 2.221818901E-06
-1.049766271E-05 7.436015325E-06 1.498298235E-06 3.873699663E-06-8.076189028E-06
 5.604664006E-06-8.348755678E-06 1.854472937E-05 9.338495793E-06-1.210305717E-05
 2.597029086E-05 6.450464447E-06-1.504792557E-05-9.249585695E-06-2.982402495E-05
 6.723028664E-06-3.610707048E-05 3.893974547E-05-9.935098543E-07 1.300871908E-05
-4.779139579E-06 1.435874141E-05 8.035682876E-06-1.563923517E-05-1.668900369E-06
-7.185579101E-06 8.714050993E-06 8.041827621E-06 2.622290330E-05-3.108356407E-07
-6.026112857E-05 2.677502287E-05-2.085698188E-05
 2.440476263E+00 1.696228403E+00 3.410396302E+00
 ......END OF GEOMETRY SEARCH......
 STEP CPU TIME =     0.16 TOTAL CPU TIME =    41537.2 (  692.3 MIN)
 TOTAL WALL CLOCK TIME=   100012.6 SECONDS, CPU UTILIZATION IS  41.53%
     1294137  WORDS OF DYNAMIC MEMORY USED
 EXECUTION OF GAMESS TERMINATED NORMALLY Fri Oct 12 00:39:17 2007
 DDI: 262808 bytes (0.3 MB / 0 MWords) used by master data server.

 ----------------------------------------
 CPU timing information for all processes
 ========================================
 0: 39156.359000 + 2381.031000 = 41537.390000
 1: 0.015000 + 0.031000 = 0.046000
 ----------------------------------------
 ddikick.x: exited gracefully.
----- accounting info -----
```

3-(dimethylazinoyl)propanoic acid (neutral gauche)

```
 Distributed Data Interface kickoff program.
 Initiating 1 compute processes on 1 nodes to run the following command:
 C:\WinGAMESS/gamess.06.exe neutral-gauche02

          ***************************************************
          *         GAMESS VERSION =  7 SEP 2006 (R4)       *
          *             FROM IOWA STATE UNIVERSITY          *
          * M.W.SCHMIDT, K.K.BALDRIDGE, J.A.BOATZ, S.T.ELBERT, *
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     PENNSYLVANIA STATE UNIVERSITY:
          TZVETELIN IORDANOV, CHET SWALINA, SHARON HAMMES-SCHIFFER

 EXECUTION OF GAMESS BEGUN Mon Oct 15 10:06:58 2007

            ECHO OF THE FIRST FEW INPUT CARDS -
 INPUT CARD> $CONTRL RUNTYP=OPTIMIZE $END
 INPUT CARD> $DFT DFTTYP=B3LYP $END
```

```
INPUT CARD> $BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.T. $END
INPUT CARD> $SYSTEM BALTYP=LOOP $END
INPUT CARD> $STATPT NSTEP=50 $END
INPUT CARD> $SYSTEM TIMLIM=6000 MWORDS=62.50 $END
INPUT CARD>
INPUT CARD> $DATA
INPUT CARD>untitled
INPUT CARD>C1
INPUT CARD> C           6.0  -0.0980361730   0.8767927134   0.3620166293
INPUT CARD> C           6.0  -1.4903731005   0.2882559694   0.6254839849
INPUT CARD> C           6.0  -2.4240697524   0.2204469833  -0.6004385108
INPUT CARD> N           7.0   0.9470490665  -0.1432513505  -0.0782238777
INPUT CARD> C           6.0   2.1421889541   0.5944813709  -0.6092892605
INPUT CARD> C           6.0   1.3688098831  -1.0028979959   1.0795299459
INPUT CARD> O           8.0   0.4647613910  -0.9698226247  -1.0779902949
INPUT CARD> O           8.0  -3.5606413018   0.6495420668  -0.5354783164
INPUT CARD> O           8.0  -1.9107891608  -0.3230716814  -1.6951318350
INPUT CARD> H           1.0   0.2964517034   1.3616963595   1.2600725033
INPUT CARD> H           1.0  -0.1397184531   1.6192980033  -0.4375872455
INPUT CARD> H           1.0  -1.9959364061   0.9167692221   1.3617570126
INPUT CARD> H           1.0  -1.4175195257  -0.7142425690   1.0570524430
INPUT CARD> H           1.0   2.8803027708  -0.1508148346  -0.9028860057
INPUT CARD> H           1.0   2.5455814519   1.2715631504   0.1499788615
INPUT CARD> H           1.0   1.8156990778   1.1460873443  -1.4898716754
INPUT CARD> H           1.0   2.0879822369  -1.7241491164   0.6932880429
INPUT CARD> H           1.0   0.4913495551  -1.5317912065   1.4451945232
INPUT CARD> H           1.0   1.8101322713  -0.3886777378   1.8703277852
INPUT CARD> H           1.0  -0.9439904884  -0.6232690665  -1.5156657100
INPUT CARD> $END

         NSERCH= 10     ENERGY=    -477.2893017

                                 ------------------------
                                 GRADIENT (HARTREE/BOHR)
                                 ------------------------
       ATOM     ZNUC        DE/DX         DE/DY         DE/DZ
------------------------------------------------------------------
 1  C            6.0    -0.0000180    -0.0000006    -0.0000231
 2  C            6.0     0.0000189    -0.0000051     0.0000296
 3  C            6.0    -0.0000443     0.0000353     0.0000000
 4  N            7.0     0.0000633    -0.0000839     0.0000083
 5  C            6.0     0.0000168     0.0000415     0.0000286
 6  C            6.0     0.0000006     0.0000445     0.0000156
 7  O            8.0     0.0000219    -0.0000007     0.0000033
 8  O            8.0     0.0000324    -0.0000265    -0.0000131
 9  O            8.0    -0.0000212     0.0000256    -0.0000073
10  H            1.0    -0.0000006     0.0000083     0.0000075
11  H            1.0    -0.0000143     0.0000156     0.0000147
12  H            1.0    -0.0000103     0.0000005    -0.0000075
13  H            1.0    -0.0000062    -0.0000050     0.0000180
14  H            1.0    -0.0000092    -0.0000120    -0.0000005
15  H            1.0     0.0000037     0.0000013    -0.0000048
16  H            1.0     0.0000099    -0.0000102    -0.0000201
17  H            1.0    -0.0000116    -0.0000037    -0.0000181
18  H            1.0    -0.0000025    -0.0000074    -0.0000183
19  H            1.0    -0.0000041     0.0000049    -0.0000011
20  H            1.0    -0.0000251    -0.0000225    -0.0000115
```

```
         MAXIMUM GRADIENT =  0.0000839    RMS GRADIENT = 0.0000222

     ***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF ALL ATOMS ARE (ANGS)
  ATOM   CHARGE       X              Y              Z
------------------------------------------------------------
C           6.0  -0.0997495975   0.8777186506   0.3583160525
C           6.0  -1.4912978098   0.2893118501   0.6266713653
C           6.0  -2.4265714565   0.2217143422  -0.5960632399
N           7.0   0.9469212986  -0.1451633432  -0.0760698789
C           6.0   2.1441716197   0.5872801723  -0.6105320129
C           6.0   1.3694359144  -1.0011582936   1.0831814787
O           8.0   0.4619603747  -0.9764929701  -1.0720673311
O           8.0  -3.5765177394   0.6117139281  -0.5173466578
O           8.0  -1.9011060425  -0.2825219711  -1.7037987389
H           1.0   0.2945927468   1.3730852225   1.2510656609
H           1.0  -0.1443684891   1.6118906026  -0.4494819503
H           1.0  -1.9950003766   0.9163081268   1.3662271998
H           1.0  -1.4203198607  -0.7160568660   1.0562405307
H           1.0   2.8802769078  -0.1632016251  -0.8968437664
H           1.0   2.5499644574   1.2668989055   0.1450314823
H           1.0   1.8210356388   1.1332594755  -1.4959034541
H           1.0   2.0989663299  -1.7125390148   0.6992747925
H           1.0   0.4957589042  -1.5423750586   1.4402838672
H           1.0   1.7984064993  -0.3852617093   1.8793797550
H           1.0  -0.9373253196  -0.5914654245  -1.5254261548

         TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS
      ATOM         MULL.POP.    CHARGE          LOW.POP.     CHARGE
   1 C             6.112397   -0.112397         6.213032   -0.213032
   2 C             6.368697   -0.368697         6.289760   -0.289760
   3 C             5.552663    0.447337         5.790181    0.209819
   4 N             7.496688   -0.496688         7.129152   -0.129152
   5 C             6.196612   -0.196612         6.302056   -0.302056
   6 C             6.239699   -0.239699         6.300342   -0.300342
   7 O             8.292580   -0.292580         8.585286   -0.585286
   8 O             8.475382   -0.475382         8.359546   -0.359546
   9 O             8.490421   -0.490421         8.352078   -0.352078
  10 H             0.838097    0.161903         0.806348    0.193652
  11 H             0.818435    0.181565         0.790274    0.209726
  12 H             0.817159    0.182841         0.797238    0.202762
  13 H             0.826249    0.173751         0.796043    0.203957
  14 H             0.814428    0.185572         0.797947    0.202053
  15 H             0.838131    0.161869         0.813708    0.186292
  16 H             0.810225    0.189775         0.795770    0.204230
  17 H             0.810355    0.189645         0.795567    0.204433
  18 H             0.820847    0.179153         0.797634    0.202366
  19 H             0.840685    0.159315         0.813794    0.186206
  20 H             0.540251    0.459749         0.674243    0.325757

         -------------------------------
         BOND ORDER AND VALENCE ANALYSIS     BOND ORDER THRESHOLD=0.050
         -------------------------------

                  BOND                          BOND                          BOND
 ATOM PAIR DIST  ORDER       ATOM PAIR DIST  ORDER       ATOM PAIR DIST  ORDER
   1   2  1.534  0.952         1   3  2.599 -0.058         1   4  1.527  0.773
   1   5  2.461 -0.074         1   9  2.974  0.062         1  10  1.094  0.938
```

```
   1  11  1.092  0.960        2   3  1.541  1.018        2   9  2.434 -0.095
   2  12  1.093  0.932        2  13  1.096  0.935        3   8  1.217  1.871
   3   9  1.326  1.159        4   5  1.502  0.807        4   6  1.502  0.844
   4   7  1.385  1.606        5   6  2.448 -0.064        5   7  2.343 -0.076
   5  14  1.090  0.966        5  15  1.094  0.939        5  16  1.089  0.970
   6   7  2.339 -0.075        6  17  1.089  0.963        6  18  1.088  0.960
   6  19  1.094  0.951        7  20  1.520  0.168        9  20  1.028  0.584

                     TOTAL       BONDED        FREE
     ATOM           VALENCE     VALENCE     VALENCE
   1 C                3.480       3.480       0.000
   2 C                3.736       3.736       0.000
   3 C                3.975       3.975       0.000
   4 N                4.049       4.049       0.000
   5 C                3.432       3.432       0.000
   6 C                3.516       3.516       0.000
   7 O                1.705       1.705       0.000
   8 O                1.824       1.824       0.000
   9 O                1.734       1.734       0.000
  10 H                0.939       0.939       0.000
  11 H                0.935       0.935       0.000
  12 H                0.937       0.937       0.000
  13 H                0.940       0.940       0.000
  14 H                0.939       0.939       0.000
  15 H                0.937       0.937       0.000
  16 H                0.938       0.938       0.000
  17 H                0.938       0.938       0.000
  18 H                0.945       0.945       0.000
  19 H                0.938       0.938       0.000
  20 H                0.797       0.797       0.000

         ---------------------
         ELECTROSTATIC MOMENTS
         ---------------------

POINT   1           X           Y           Z (BOHR)    CHARGE
              -0.930325    0.007271   -0.566659        0.00 (A.U.)
        DX          DY          DZ         /D/  (DEBYE)
    7.958777    1.564047    5.075952    9.568368
...... END OF PROPERTY EVALUATION ......
STEP CPU TIME =     2.83 TOTAL CPU TIME =    11768.0 (  196.1 MIN)
TOTAL WALL CLOCK TIME=    23555.4 SECONDS, CPU UTILIZATION IS  49.96%
 $VIB
         IVIB=   0 IATOM=   0 ICOORD=   0 E=     -477.2893017386
-1.804226268E-05-6.218527076E-07-2.310225745E-05 1.892639768E-05-5.101249344E-06
 2.959143467E-05-4.427212516E-05 3.526328910E-05 2.949767760E-08 6.331635928E-05
-8.388316631E-05 8.298900602E-06 1.678017449E-05 4.152884400E-05 2.859810330E-05
 6.498185208E-07 4.448348112E-05 1.555986505E-05 2.190989490E-05-7.135937337E-07
 3.288421248E-06 3.235609761E-05-2.649832882E-05-1.307566709E-05-2.124756534E-05
 2.563643121E-05-7.312032738E-06-5.612028019E-07 8.334503067E-06 7.472123118E-06
-1.433700815E-05 1.564321675E-05 1.466205969E-05-1.028468806E-05 5.430109878E-07
-7.450434152E-06-6.209419303E-06-4.973496256E-06 1.799095833E-05-9.235543627E-06
-1.203632585E-05-5.321489629E-07 3.687524672E-06 1.250028267E-06-4.842636592E-06
 9.903266118E-06-1.019883602E-05-2.013762532E-05-1.164462258E-05-3.674922627E-06
-1.813748119E-05-2.502284954E-06-7.396953795E-06-1.831687910E-05-4.111445838E-06
 4.912353455E-06-1.074505948E-06-2.508136476E-05-2.249643250E-05-1.150969514E-05
 7.958777405E+00 1.564046760E+00 5.075951871E+00
......END OF GEOMETRY SEARCH......
```

```
 STEP CPU TIME =     0.14 TOTAL CPU TIME =    11768.2 (  196.1 MIN)
 TOTAL WALL CLOCK TIME=    23555.6 SECONDS, CPU UTILIZATION IS  49.96%
     1279627  WORDS OF DYNAMIC MEMORY USED
 EXECUTION OF GAMESS TERMINATED NORMALLY Mon Oct 15 16:39:34 2007
 DDI: 262808 bytes (0.3 MB / 0 MWords) used by master data server.

 ----------------------------------------
 CPU timing information for all processes
 ========================================
 0: 11084.015000 + 684.328000 = 11768.343000
 1: 0.015000 + 0.062000 = 0.077000
 ----------------------------------------
 ddikick.x: exited gracefully.
----- accounting info -----
```

3-(dimethylazinoyl)propanoic acid (neutral non hydrogen bonded)

```
 Distributed Data Interface kickoff program.
 Initiating 1 compute processes on 1 nodes to run the following command:
 C:\WinGAMESS/gamess.06.exe neutral-gauche-nohbd01

          ***************************************************
          *         GAMESS VERSION =  7 SEP 2006 (R4)       *
          *             FROM IOWA STATE UNIVERSITY          *
          * M.W.SCHMIDT, K.K.BALDRIDGE, J.A.BOATZ, S.T.ELBERT, *
          *   M.S.GORDON, J.H.JENSEN, S.KOSEKI, N.MATSUNAGA,   *
          *           K.A.NGUYEN, S.J.SU, T.L.WINDUS,         *
          *       TOGETHER WITH M.DUPUIS, J.A.MONTGOMERY      *
          *         J.COMPUT.CHEM.  14, 1347-1363(1993)       *
          ****************** PC-UNIX VERSION *****************

     SINCE 1993, STUDENTS AND POSTDOCS WORKING AT IOWA STATE UNIVERSITY
     AND ALSO IN THEIR VARIOUS JOBS AFTER LEAVING ISU HAVE MADE IMPORTANT
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     WEI CHEN, CHEOL HO CHOI, PAUL DAY, TIM DUDLEY, DMITRI FEDOROV,
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          KAROL KOWALSKI, MARTA WLOCH, PIOTR PIECUCH
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     PENNSYLVANIA STATE UNIVERSITY:
          TZVETELIN IORDANOV, CHET SWALINA, SHARON HAMMES-SCHIFFER

 EXECUTION OF GAMESS BEGUN Tue Oct 23 11:07:08 2007

            ECHO OF THE FIRST FEW INPUT CARDS -
 INPUT CARD> $CONTRL RUNTYP=OPTIMIZE $END
 INPUT CARD> $DFT DFTTYP=B3LYP $END
```

```
INPUT CARD> $BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.T. $END
INPUT CARD> $SYSTEM BALTYP=LOOP $END
INPUT CARD> $STATPT NSTEP=50 $END
INPUT CARD> $SYSTEM TIMLIM=6000 MWORDS=62.50 $END
INPUT CARD>
INPUT CARD> $DATA
INPUT CARD>untitled
INPUT CARD>C1
INPUT CARD>C        6.0       -0.050025        1.018047        0.162065
INPUT CARD>C        6.0       -1.440844        0.561881        0.666493
INPUT CARD>C        6.0       -2.199444       -0.215081       -0.373511
INPUT CARD>N        7.0        0.863259       -0.090267       -0.218695
INPUT CARD>C        6.0        2.204571        0.465483       -0.522987
INPUT CARD>C        6.0        1.010108       -1.068493        0.883782
INPUT CARD>O        8.0        0.468020       -0.693649       -1.069915
INPUT CARD>O        8.0       -3.193021       -0.967585        0.096714
INPUT CARD>O        8.0       -2.074528        0.005964       -1.567489
INPUT CARD>H        1.0        0.416824        1.609563        0.964933
INPUT CARD>H        1.0       -0.210125        1.686383       -0.698664
INPUT CARD>H        1.0       -2.025817        1.462945        0.905472
INPUT CARD>H        1.0       -1.346719       -0.034301        1.585638
INPUT CARD>H        1.0        2.828998       -0.292117       -1.021922
INPUT CARD>H        1.0        2.706831        0.777807        0.405384
INPUT CARD>H        1.0        2.125371        1.341035       -1.185728
INPUT CARD>H        1.0        1.899534       -1.696081        0.719624
INPUT CARD>H        1.0        0.134124       -1.733661        0.938020
INPUT CARD>H        1.0        1.123590       -0.551205        1.848595
INPUT CARD>H        1.0       -3.682927       -1.358378       -0.617589
INPUT CARD> $END

         NSERCH= 41     ENERGY=    -477.2785307

                                 ----------------------
                                 GRADIENT (HARTREE/BOHR)
                                 ----------------------
       ATOM     ZNUC       DE/DX         DE/DY         DE/DZ
------------------------------------------------------------
 1  C            6.0     0.0000121     0.0000523    -0.0000050
 2  C            6.0    -0.0000299     0.0000271     0.0000061
 3  C            6.0    -0.0000293    -0.0000145    -0.0000338
 4  N            7.0     0.0000455     0.0000066    -0.0000311
 5  C            6.0    -0.0000576    -0.0000451     0.0000280
 6  C            6.0     0.0000053    -0.0000239     0.0000672
 7  O            8.0     0.0000017     0.0000136     0.0000030
 8  O            8.0     0.0000143     0.0000220    -0.0000271
 9  O            8.0     0.0000126    -0.0000322     0.0000591
10  H            1.0     0.0000001    -0.0000063    -0.0000079
11  H            1.0    -0.0000008     0.0000026    -0.0000022
12  H            1.0     0.0000062    -0.0000145    -0.0000130
13  H            1.0     0.0000018    -0.0000031    -0.0000036
14  H            1.0     0.0000219    -0.0000096    -0.0000279
15  H            1.0    -0.0000012     0.0000023     0.0000383
16  H            1.0    -0.0000208     0.0000261    -0.0000269
17  H            1.0    -0.0000104    -0.0000014     0.0000121
18  H            1.0     0.0000284     0.0000290    -0.0000144
19  H            1.0    -0.0000128    -0.0000274    -0.0000347
20  H            1.0     0.0000128    -0.0000035     0.0000137
```

```
         MAXIMUM GRADIENT =  0.0000672    RMS GRADIENT = 0.0000249

     ***** EQUILIBRIUM GEOMETRY LOCATED *****
COORDINATES OF ALL ATOMS ARE (ANGS)
  ATOM   CHARGE       X              Y              Z
------------------------------------------------------------
C           6.0  -0.1038411745   0.9221082699   0.4095613859
C           6.0  -1.5038165086   0.3910259843   0.6822126113
C           6.0  -2.2500747057   0.1032652362  -0.6065121317
N           7.0   0.8403756776  -0.2111812771   0.0096768562
C           6.0   2.0091545456   0.3772151612  -0.7303719438
C           6.0   1.3475665924  -0.9188043997   1.2378213008
O           8.0   0.1856733542  -1.1044845266  -0.7949899971
O           8.0  -3.0287070734  -0.9977147785  -0.5150642125
O           8.0  -2.2534705009   0.8359275395  -1.5750349990
H           1.0   0.3167505833   1.4398433852   1.2777673553
H           1.0  -0.1443751088   1.6074525671  -0.4390730677
H           1.0  -2.0653918493   1.1798208126   1.2014227213
H           1.0  -1.5057592621  -0.4919388151   1.3228057265
H           1.0   2.6912095815  -0.4411696761  -0.9598131699
H           1.0   2.5068887244   1.1444018728  -0.1273253580
H           1.0   1.6173582265   0.7946643517  -1.6570686156
H           1.0   1.9482256262  -1.7577486032   0.8882385144
H           1.0   0.4866212848  -1.3021034950   1.7833942525
H           1.0   1.9387155730  -0.2437176446   1.8653084259
H           1.0  -3.4753235863  -1.0985719646  -1.3727356547

          TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS
      ATOM         MULL.POP.    CHARGE          LOW.POP.     CHARGE
   1 C             6.162516   -0.162516         6.217289   -0.217289
   2 C             6.227725   -0.227725         6.271810   -0.271810
   3 C             5.618649    0.381351         5.766620    0.233380
   4 N             7.459641   -0.459641         7.124979   -0.124979
   5 C             6.229041   -0.229041         6.311241   -0.311241
   6 C             6.256433   -0.256433         6.313816   -0.313816
   7 O             8.242552   -0.242552         8.577154   -0.577154
   8 O             8.418361   -0.418361         8.343580   -0.343580
   9 O             8.448560   -0.448560         8.364198   -0.364198
  10 H             0.856330    0.143670         0.811080    0.188920
  11 H             0.811734    0.188266         0.783449    0.216551
  12 H             0.829130    0.170870         0.801889    0.198111
  13 H             0.823351    0.176649         0.793817    0.206183
  14 H             0.824403    0.175597         0.802662    0.197338
  15 H             0.849257    0.150743         0.818675    0.181325
  16 H             0.808741    0.191259         0.795144    0.204856
  17 H             0.814273    0.185727         0.798348    0.201652
  18 H             0.830024    0.169976         0.801050    0.198950
  19 H             0.850784    0.149216         0.819374    0.180626
  20 H             0.638497    0.361503         0.683824    0.316176

          ------------------------------
          BOND ORDER AND VALENCE ANALYSIS     BOND ORDER THRESHOLD=0.050
          ------------------------------

                    BOND                          BOND                          BOND
 ATOM PAIR DIST   ORDER       ATOM PAIR DIST   ORDER       ATOM PAIR DIST   ORDER
   1   2  1.522  0.992         1   4  1.528  0.722         1   5  2.462 -0.070
   1  10  1.095  0.931         1  11  1.092  0.986         2   3  1.517  0.976
```

```
   2   8  2.385 -0.161        2   9  2.420 -0.132        2  12  1.099  0.910
   2  13  1.091  0.950        3   7  2.725  0.067        3   8  1.352  1.171
   3   9  1.214  1.898        4   5  1.503  0.796        4   6  1.505  0.833
   4   7  1.369  1.699        5   6  2.448 -0.059        5   7  2.350 -0.052
   5  14  1.090  0.971        5  15  1.095  0.943        5  16  1.089  0.976
   6   7  2.349 -0.051        6  17  1.089  0.969        6  18  1.089  0.963
   6  19  1.095  0.953        8  20  0.972  0.804
```

	ATOM	TOTAL VALENCE	BONDED VALENCE	FREE VALENCE
1	C	3.535	3.535	0.000
2	C	3.490	3.490	0.000
3	C	4.103	4.103	0.000
4	N	3.979	3.979	0.000
5	C	3.475	3.475	0.000
6	C	3.547	3.547	0.000
7	O	1.661	1.661	0.000
8	O	1.775	1.775	0.000
9	O	1.789	1.789	0.000
10	H	0.940	0.940	0.000
11	H	0.941	0.941	0.000
12	H	0.935	0.935	0.000
13	H	0.941	0.941	0.000
14	H	0.941	0.941	0.000
15	H	0.939	0.939	0.000
16	H	0.938	0.938	0.000
17	H	0.938	0.938	0.000
18	H	0.945	0.945	0.000
19	H	0.939	0.939	0.000
20	H	0.869	0.869	0.000

```
         ---------------------
         ELECTROSTATIC MOMENTS
         ---------------------

POINT   1           X           Y           Z (BOHR)    CHARGE
              -1.014116   -0.168645   -0.430081        0.00 (A.U.)
        DX          DY          DZ         /D/  (DEBYE)
    2.654448    1.854546    3.937962    5.098331
...... END OF PROPERTY EVALUATION ......
STEP CPU TIME =     2.86 TOTAL CPU TIME =    43569.7 (  726.2 MIN)
TOTAL WALL CLOCK TIME=    99826.1 SECONDS, CPU UTILIZATION IS  43.65%
 $VIB
         IVIB=   0 IATOM=   0 ICOORD=   0 E=     -477.2785306728
 1.211035760E-05 5.229465246E-05-5.009531335E-06-2.987412870E-05 2.712589682E-05
 6.126000852E-06-2.927914856E-05-1.450954855E-05-3.377164398E-05 4.549480633E-05
 6.594732345E-06-3.113273460E-05-5.761112951E-05-4.509417172E-05 2.804269973E-05
 5.302098726E-06-2.391632645E-05 6.719445368E-05 1.723076222E-06 1.361223282E-05
 3.035204354E-06 1.434077677E-05 2.195379280E-05-2.705569394E-05 1.263536740E-05
-3.223911951E-05 5.911012860E-05 1.359198247E-07-6.302542073E-06-7.917349673E-06
-7.962512148E-07 2.618123624E-06-2.238643790E-06 6.236079402E-06-1.450436877E-05
-1.304569374E-05 1.769257009E-06-3.141476126E-06-3.573389063E-06 2.186293439E-05
-9.583896916E-06-2.785392578E-05-1.205497233E-06 2.316998716E-06 3.832089380E-05
-2.076980265E-05 2.613599161E-05-2.692798803E-05-1.040731791E-05-1.436540412E-06
 1.211329520E-05 2.839691922E-05 2.898553773E-05-1.443333194E-05-1.284177032E-05
-2.738548070E-05-3.470837981E-05 1.277745319E-05-3.524487699E-06 1.372562946E-05
 2.654447863E+00 1.854545717E+00 3.937961757E+00
......END OF GEOMETRY SEARCH......
```

```
 STEP CPU TIME =     0.14 TOTAL CPU TIME =    43569.8 (  726.2 MIN)
 TOTAL WALL CLOCK TIME=    99826.3 SECONDS, CPU UTILIZATION IS  43.65%
     1279627  WORDS OF DYNAMIC MEMORY USED
 EXECUTION OF GAMESS TERMINATED NORMALLY Wed Oct 24 14:50:54 2007
 DDI: 262808 bytes (0.3 MB / 0 MWords) used by master data server.

 ----------------------------------------
 CPU timing information for all processes
 ========================================
 0: 41056.125000 + 2513.937000 = 43570.062000
 1: 0.015000 + 0.062000 = 0.077000
 ----------------------------------------
 ddikick.x: exited gracefully.
----- accounting info -----
```

3-(dimethylazinoyl)propanoic acid (deprotonated gauche)

```
 Distributed Data Interface kickoff program.
 Initiating 1 compute processes on 1 nodes to run the following command:
 C:\WinGAMESS/gamess.06.exe deprotonated-gauche02

          ***************************************************
          *         GAMESS VERSION =  7 SEP 2006 (R4)       *
          *             FROM IOWA STATE UNIVERSITY          *
          * M.W.SCHMIDT, K.K.BALDRIDGE, J.A.BOATZ, S.T.ELBERT, *
          *   M.S.GORDON, J.H.JENSEN, S.KOSEKI, N.MATSUNAGA,   *
          *           K.A.NGUYEN, S.J.SU, T.L.WINDUS,         *
          *       TOGETHER WITH M.DUPUIS, J.A.MONTGOMERY      *
          *         J.COMPUT.CHEM.  14, 1347-1363(1993)       *
          ****************** PC-UNIX VERSION *****************

     SINCE 1993, STUDENTS AND POSTDOCS WORKING AT IOWA STATE UNIVERSITY
     AND ALSO IN THEIR VARIOUS JOBS AFTER LEAVING ISU HAVE MADE IMPORTANT
     CONTRIBUTIONS TO THE CODE:
     IVANA ADAMOVIC, CHRISTINE AIKENS, YURI ALEXEEV, POOJA ARORA, ROB BELL,
     PRADIPTA BANDYOPADHYAY, JONATHAN BENTZ, BRETT BODE, GALINA CHABAN,
     WEI CHEN, CHEOL HO CHOI, PAUL DAY, TIM DUDLEY, DMITRI FEDOROV,
     GRAHAM FLETCHER, MARK FREITAG, KURT GLAESEMANN, GRANT MERRILL,
     TAKESHI NAGATA, HEATHER NETZLOFF, BOSILJKA NJEGIC, RYAN OLSON,
     MIKE PAK, JIM SHOEMAKER, LYUDMILA SLIPCHENKO, JIE SONG,
     TETSUYA TAKETSUGU, SIMON WEBB.

     ADDITIONAL CODE HAS BEEN PROVIDED BY COLLABORATORS IN OTHER GROUPS:
     IOWA STATE UNIVERSITY: JOE IVANIC, KLAUS RUEDENBERG
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          KIYOSHI YAGI, MAHITO CHIBA
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     UNIVERSITY OF PISA: BENEDETTA MENNUCCI, JACOPO TOMASI
     UNIVERSITY OF MEMPHIS: HENRY KURTZ, PRAKASHAN KORAMBATH
     UNIVERSITY OF ALBERTA: MARIUSZ KLOBUKOWSKI
     UNIVERSITY OF NEW ENGLAND: MARK SPACKMAN
     MIE UNIVERSITY: HIROAKI UMEDA
     MICHIGAN STATE UNIVERSITY:
          KAROL KOWALSKI, MARTA WLOCH, PIOTR PIECUCH
     UNIVERSITY OF SILESIA: MONIKA MUSIAL, STANISLAW KUCHARSKI
     FACULTES UNIVERSITAIRES NOTRE-DAME DE LA PAIX:
          OLIVIER QUINET, BENOIT CHAMPAGNE
     UNIVERSITY OF CALIFORNIA - SANTA BARBARA: BERNARD KIRTMAN
     INSTITUTE FOR MOLECULAR SCIENCE: KAZUYA ISHIMURA AND SHIGERU NAGASE
     UNIVERSITY OF NOTRE DAME: DAN CHIPMAN
     KYUSHU UNIVERSITY:
          FENG LONG GU, JACEK KORCHOWIEC, MARCIN MAKOWSKI, AND YURIKO AOKI
     PENNSYLVANIA STATE UNIVERSITY:
          TZVETELIN IORDANOV, CHET SWALINA, SHARON HAMMES-SCHIFFER

 EXECUTION OF GAMESS BEGUN Fri Oct 19 10:18:43 2007

            ECHO OF THE FIRST FEW INPUT CARDS -
 INPUT CARD> $CONTRL RUNTYP=OPTIMIZE $END
 INPUT CARD> $DFT DFTTYP=B3LYP $END
```

```
INPUT CARD> $BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 DIFFSP=.T. $END
INPUT CARD> $CONTRL ICHARG=-1 $END
INPUT CARD> $SYSTEM BALTYP=LOOP $END
INPUT CARD> $STATPT NSTEP=50 $END
INPUT CARD> $SYSTEM TIMLIM=6000 MWORDS=62.50 $END
INPUT CARD>
INPUT CARD> $DATA
INPUT CARD>untitled
INPUT CARD>C1
INPUT CARD> C           6.0  -0.1810166520   0.7997651477  -0.6566102173
INPUT CARD> C           6.0  -1.1108167850   0.8894789904   0.5500183372
INPUT CARD> C           6.0  -2.1012192666  -0.3185748980   0.7703266495
INPUT CARD> N           7.0   1.1293931732   0.0342924935  -0.4755601969
INPUT CARD> C           6.0   1.9805634841   0.7013875921   0.5573762191
INPUT CARD> C           6.0   0.8512149291  -1.3851546814  -0.0742662840
INPUT CARD> O           8.0   1.8267325970   0.0431679596  -1.6656009150
INPUT CARD> O           8.0  -2.5827782634  -0.3873074882   1.9325932398
INPUT CARD> O           8.0  -2.3328082235  -1.0445638232  -0.2335584009
INPUT CARD> H           1.0   0.1554317104   1.7742884481  -1.0226969869
INPUT CARD> H           1.0  -0.6930028047   0.2749022218  -1.4656362201
INPUT CARD> H           1.0  -1.7534504344   1.7754157146   0.3941210469
INPUT CARD> H           1.0  -0.5744168946   1.0801869020   1.4917818814
INPUT CARD> H           1.0   2.9343339953   0.1724635234   0.5675910653
INPUT CARD> H           1.0   1.5095361709   0.6865292604   1.5428302915
INPUT CARD> H           1.0   2.1351471887   1.7240340759   0.2101508647
INPUT CARD> H           1.0   1.8191729183  -1.8893753658  -0.0076846135
INPUT CARD> H           1.0   0.2474211715  -1.8200473790  -0.8661779706
INPUT CARD> H           1.0   0.3062398499  -1.4375739582   0.8709688279
INPUT CARD> $END

         NSERCH= 48     ENERGY=    -476.7377840

                                 ------------------------
                                 GRADIENT (HARTREE/BOHR)
                                 ------------------------
       ATOM     ZNUC        DE/DX         DE/DY         DE/DZ
------------------------------------------------------------
 1  C            6.0    -0.0000135    -0.0000102     0.0000369
 2  C            6.0    -0.0000234     0.0000695    -0.0000694
 3  C            6.0     0.0000126     0.0000091     0.0000196
 4  N            7.0    -0.0000081    -0.0000267    -0.0000011
 5  C            6.0     0.0000381     0.0000301    -0.0000046
 6  C            6.0    -0.0000366    -0.0000010     0.0000013
 7  O            8.0    -0.0000054    -0.0000063     0.0000092
 8  O            8.0    -0.0000162    -0.0000064    -0.0000088
 9  O            8.0    -0.0000084    -0.0000080     0.0000067
10  H            1.0    -0.0000181     0.0000265    -0.0000004
11  H            1.0     0.0000001    -0.0000152     0.0000047
12  H            1.0     0.0000540    -0.0000655     0.0000082
13  H            1.0     0.0000220    -0.0000307     0.0000035
14  H            1.0    -0.0000053     0.0000125    -0.0000021
15  H            1.0    -0.0000187    -0.0000044     0.0000170
16  H            1.0     0.0000101    -0.0000058     0.0000022
17  H            1.0    -0.0000063    -0.0000111    -0.0000102
18  H            1.0     0.0000175     0.0000286     0.0000209
19  H            1.0     0.0000059     0.0000152    -0.0000335

         MAXIMUM GRADIENT =  0.0000695    RMS GRADIENT = 0.0000236
```

***** EQUILIBRIUM GEOMETRY LOCATED *****

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
C	6.0	-0.1762888579	0.7946963402	-0.7847196012
C	6.0	-1.1669221962	1.0741230218	0.3523580347
C	6.0	-1.7196901960	-0.1975484132	1.0746009766
N	7.0	1.1116966525	0.0305743544	-0.4572285049
C	6.0	1.7094605807	0.5448989004	0.8220776118
C	6.0	0.8296832198	-1.4376127237	-0.3035159086
O	8.0	2.0026314820	0.2129230832	-1.4978534779
O	8.0	-1.1857602976	-0.4646091632	2.1908360149
O	8.0	-2.6004866074	-0.8411718869	0.4492729225
H	1.0	0.2084050622	1.7214525075	-1.2175637084
H	1.0	-0.6462470397	0.2153492807	-1.5826089942
H	1.0	-2.0100744949	1.5913757163	-0.1233483280
H	1.0	-0.7232132799	1.7576792533	1.0848848827
H	1.0	2.6638352934	0.0299506776	0.9411400472
H	1.0	1.0302741452	0.3522052230	1.6578393801
H	1.0	1.8917235465	1.6109931667	0.6804534816
H	1.0	1.7964920391	-1.9233290164	-0.1595776620
H	1.0	0.3927481725	-1.7750717125	-1.2430532078
H	1.0	0.1574106399	-1.6235638735	0.5359726587

TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS

	ATOM	MULL.POP.	CHARGE	LOW.POP.	CHARGE
1	C	6.119896	-0.119896	6.225802	-0.225802
2	C	6.206621	-0.206621	6.335827	-0.335827
3	C	5.824905	0.175095	5.877380	0.122620
4	N	7.442360	-0.442360	7.130671	-0.130671
5	C	6.336930	-0.336930	6.329134	-0.329134
6	C	6.248248	-0.248248	6.314722	-0.314722
7	O	8.311439	-0.311439	8.648066	-0.648066
8	O	8.552647	-0.552647	8.564548	-0.564548
9	O	8.556270	-0.556270	8.523553	-0.523553
10	H	0.842121	0.157879	0.804493	0.195507
11	H	0.841815	0.158185	0.797330	0.202670
12	H	0.865390	0.134610	0.818674	0.181326
13	H	0.866317	0.133683	0.822374	0.177626
14	H	0.853348	0.146652	0.812940	0.187060
15	H	0.783615	0.216385	0.782066	0.217934
16	H	0.852666	0.147334	0.812307	0.187693
17	H	0.858453	0.141547	0.815029	0.184971
18	H	0.846209	0.153791	0.805665	0.194335
19	H	0.790750	0.209250	0.779419	0.220581

BOND ORDER AND VALENCE ANALYSIS BOND ORDER THRESHOLD=0.050

ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER	ATOM	PAIR	DIST	BOND ORDER
1	2	1.534	0.827	1	4	1.533	0.769	1	6	2.495	-0.070
1	10	1.093	0.997	1	11	1.092	0.997	2	3	1.563	0.824
2	8	2.398	-0.188	2	9	2.394	-0.192	2	12	1.098	0.940
2	13	1.096	0.993	3	8	1.266	1.785	3	9	1.257	1.819

```
   4   5  1.503  0.800        4   6  1.503  0.787        4   7  1.382  1.655
   5   6  2.444 -0.059        5  14  1.091  0.983        5  15  1.094  0.933
   5  16  1.091  0.985        6   8  3.351 -0.071        6  17  1.091  0.991
   6  18  1.090  0.987        6  19  1.091  0.926
```

	ATOM	TOTAL VALENCE	BONDED VALENCE	FREE VALENCE
1	C	3.338	3.338	0.000
2	C	3.117	3.117	0.000
3	C	4.418	4.418	0.000
4	N	3.915	3.915	0.000
5	C	3.581	3.581	0.000
6	C	3.421	3.421	0.000
7	O	1.587	1.587	0.000
8	O	1.536	1.536	0.000
9	O	1.594	1.594	0.000
10	H	0.943	0.943	0.000
11	H	0.945	0.945	0.000
12	H	0.943	0.943	0.000
13	H	0.939	0.939	0.000
14	H	0.948	0.948	0.000
15	H	0.932	0.932	0.000
16	H	0.947	0.947	0.000
17	H	0.948	0.948	0.000
18	H	0.949	0.949	0.000
19	H	0.938	0.938	0.000

```
         ---------------------
         ELECTROSTATIC MOMENTS
         ---------------------

POINT   1           X           Y           Z (BOHR)    CHARGE
              -0.206737   -0.082090    0.377412       -1.00 (A.U.)
        DX          DY          DZ         /D/  (DEBYE)
    3.262513    2.433872   -0.575281    4.110800
...... END OF PROPERTY EVALUATION ......
STEP CPU TIME =     2.72 TOTAL CPU TIME =    52066.8 (  867.8 MIN)
TOTAL WALL CLOCK TIME=    98049.3 SECONDS, CPU UTILIZATION IS  53.10%
 $VIB
         IVIB=   0 IATOM=   0 ICOORD=   0 E=     -476.7377839590
-1.349883828E-05-1.020714856E-05 3.687495596E-05-2.343239039E-05 6.947157081E-05
-6.941019320E-05 1.255554998E-05 9.069097020E-06 1.959266895E-05-8.084593105E-06
-2.667796412E-05-1.102069345E-06 3.805012026E-05 3.006661153E-05-4.578552845E-06
-3.655905502E-05-1.010444841E-06 1.335607534E-06-5.351896415E-06-6.338309984E-06
 9.225319504E-06-1.620397965E-05-6.448192863E-06-8.757562627E-06-8.405042404E-06
-8.022648325E-06 6.653720994E-06-1.810757961E-05 2.647547222E-05-4.159165522E-07
 5.085336868E-08-1.519832808E-05 4.659564611E-06 5.396080516E-05-6.554763164E-05
 8.170521250E-06 2.199762693E-05-3.067333890E-05 3.514090403E-06-5.348137842E-06
 1.248401106E-05-2.100221252E-06-1.874387164E-05-4.406913824E-06 1.695691452E-05
 1.008580950E-05-5.753888641E-06 2.194229456E-06-6.340409003E-06-1.114478127E-05
-1.017286572E-05 1.747638182E-05 2.864173875E-05 2.085463001E-05 5.898646352E-06
 1.522108967E-05-3.349484165E-05
 3.262512947E+00 2.433872183E+00-5.752810650E-01
......END OF GEOMETRY SEARCH......
STEP CPU TIME =     0.13 TOTAL CPU TIME =    52067.0 (  867.8 MIN)
TOTAL WALL CLOCK TIME=    98049.5 SECONDS, CPU UTILIZATION IS  53.10%
    1265553  WORDS OF DYNAMIC MEMORY USED
EXECUTION OF GAMESS TERMINATED NORMALLY Sat Oct 20 13:32:53 2007
```

```
 DDI: 262808 bytes (0.3 MB / 0 MWords) used by master data server.

 ----------------------------------------
 CPU timing information for all processes
 ========================================
 0: 48978.968000 + 3088.203000 = 52067.171000
 1: 0.062000 + 0.015000 = 0.077000
 ----------------------------------------
 ddikick.x: exited gracefully.
----- accounting info -----
```

Altona Equations: 3-(Dimethylazinoyl)propanoic acid

Conjugate Acid

60˚ Dihedral Angle

H_2O, Methanol, Ethanol, Isopropyl Alchol, and *tert*-Butyl Alcohol
$J_{13} = 4.00133 \times (\text{Fraction Gauche}) + 4.11459$
$J_{14} = -10.1093 \times (\text{Fraction Gauche}) + 13.5217$

Ethylene Carbonate
$J_{13} = 3.98619 \times (\text{Fraction Gauche}) + 4.11654$
$J_{14} = -10.0935 \times (\text{Fraction Gauche}) + 13.503$

DMSO
$J_{13} = 3.82311 \times (\text{Fraction Gauche}) + 4.16006$
$J_{14} = -10.0437 \times (\text{Fraction Gauche}) + 13.4046$

Acetonitrile
$J_{13} = 3.9455 \times (\text{Fraction Gauche}) + 4.12737$
$J_{14} = -10.0799 \times (\text{Fraction Gauche}) + 13.4776$

65.0˚ Dihedral Angle

H_2O and Ethanol
$J_{13} = 4.06342 \times (\text{Fraction Gauche}) + 4.5009$
$J_{14} = -10.9697 \times (\text{Fraction Gauche}) + 13.6375$

Methanol
$J_{13} = 4.39077 \times (\text{Fraction Gauche}) + 4.08972$
$J_{14} = -10.9236 \times (\text{Fraction Gauche}) + 13.5687$

Isopropyl Alcohol
$J_{13} = 4.3246 \times (\text{Fraction Gauche}) + 4.10576$
$J_{14} = -10.8984 \times (\text{Fraction Gauche}) + 13.5289$

tert-Butyl Alcohol and DMSO
$J_{13} = 4.10117 \times (\text{Fraction Gauche}) + 4.16006$
$J_{14} = -10.828 \times (\text{Fraction Gauche}) + 13.4046$

Ethylene Carbonate
$J_{13} = 4.27978 \times (\text{Fraction Gauche}) + 4.11654$
$J_{14} = -10.8826 \times (\text{Fraction Gauche}) + 13.503$

Acetonitrile
$J_{13} = 4.23521 \times (\text{Fraction Gauche}) + 4.12737$
$J_{14} = -10.8677 \times (\text{Fraction Gauche}) + 13.4776$

Neutral

60˚ Dihedral Angle

H_2O, Methanol, Ethanol, Isopropyl Alcohol, and *tert*-Butyl Alcohol
$J_{13} = 3.96 \times (\text{Fraction Gauche}) + 4.118$
$J_{14} = -10.054 \times (\text{Fraction Gauche}) + 13.46$

Ethylene Carbonate
$J_{13} = 3.98619 \times (\text{Fraction Gauche}) + 4.11654$
$J_{14} = -10.0935 \times (\text{Fraction Gauche}) + 13.503$

DMSO
$J_{13} = 3.82311 \times (\text{Fraction Gauche}) + 4.16006$
$J_{14} = -10.0437 \times (\text{Fraction Gauche}) + 13.4046$

Acetonitrile
$J_{13} = 3.9455 \times (\text{Fraction Gauche}) + 4.12737$
$J_{14} = -10.0799 \times (\text{Fraction Gauche}) + 13.4776$

88.8˚ Dihedral Angle

H_2O and Ethanol
$J_{13} = 5.20023 \times (\text{Fraction Gauche}) + 4.06342$
$J_{14} = -10.9697 \times (\text{Fraction Gauche}) + 13.6375$

Methanol
$J_{13} = 5.06617 \times (\text{Fraction Gauche}) + 4.08972$
$J_{14} = -12.7391 \times (\text{Fraction Gauche}) + 13.5687$

Isopropyl Alcohol
$J_{13} = 4.98523 \times (\text{Fraction Gauche}) + 4.10576$
$J_{14} = -12.7084 \times (\text{Fraction Gauche}) + 13.5289$

tert-Butyl Alcohol and DMSO
$J_{13} = 4.71376 \times (\text{Fraction Gauche}) + 4.16006$
$J_{14} = -12.6227 \times (\text{Fraction Gauche}) + 13.4046$

Ethylene Carbonate
$J_{13} = 4.9311 \times (\text{Fraction Gauche}) + 4.11654$
$J_{14} = -12.6892 \times (\text{Fraction Gauche}) + 13.503$

Acetonitrile
$J_{13} = 4.87686 \times (\text{Fraction Gauche}) + 4.12737$
$J_{14} = -12.671 \times (\text{Fraction Gauche}) + 13.4776$

Conjugate Base

60˚ Dihedral Angle

H_2O and Ethanol
$J_{13} = 4.87652 \times (\text{Fraction Gauche}) + 4.07452$
$J_{14} = -12.0854 \times (\text{Fraction Gauche}) + 13.5451$

Methanol
$J_{13} = 4.14726 \times (\text{Fraction Gauche}) + 4.08251$
$J_{14} = -10.1945 \times (\text{Fraction Gauche}) + 13.6437$

Isopropyl Alcohol
$J_{13} = 4.08653 \times (\text{Fraction Gauche}) + 4.09855$
$J_{14} = -10.1714 \times (\text{Fraction Gauche}) + 13.6038$

tert-Butyl Alcohol
$J_{13} = 3.88283 \times (\text{Fraction Gauche}) + 4.15284$
$J_{14} = -10.1071 \times (\text{Fraction Gauche}) + 13.4795$

Ethylene Carbonate
$J_{13} = 3.92423 \times (\text{Fraction Gauche}) + 4.12525$
$J_{14} = -10.0314 \times (\text{Fraction Gauche}) + 13.429$

DMSO
$J_{13} = 3.76115 \times (\text{Fraction Gauche}) + 4.16876$
$J_{14} = -9.98151 \times (\text{Fraction Gauche}) + 13.3305$

Acetonitrile
$J_{13} = 3.88354 \times (\text{Fraction Gauche}) + 4.13607$
$J_{14} = -10.0177 \times (\text{Fraction Gauche}) + 13.4036$

59.2˚ Dihedral Angle

H_2O
$J_{13} = 4.05775 \times (\text{Fraction Gauche}) + 4.07452$
$J_{14} = -9.95992 \times (\text{Fraction Gauche}) + 13.5451$

Methanol
$J_{13} = 4.09407 \times (\text{Fraction Gauche}) + 4.08251$
$J_{14} = -10.0572 \times (\text{Fraction Gauche}) + 13.6437$

Ethanol
$J_{13} = 4.19302 \times (\text{Fraction Gauche}) + 4.0562$
$J_{14} = -10.0986 \times (\text{Fraction Gauche}) + 13.7124$

Isopropyl Alchol
$J_{13} = 4.03432 \times (\text{Fraction Gauche}) + 4.09855$

J_{14} = -10.0345 × (Fraction Gauche) + 13.6038

tert-Butyl Alcohol
J_{13} = 3.83394 × (Fraction Gauche) + 4.15284
J_{14} = -9.9713 × (Fraction Gauche) + 13.4795

Ethylene Carbonate
J_{13} = 3.87466 × (Fraction Gauche) + 4.12525
J_{14} = -9.89677× (Fraction Gauche) + 13.429

DMSO
J_{13} = 3.71424 × (Fraction Gauche) + 4.16876
J_{14} = -9.84772× (Fraction Gauche) + 13.3305

Acetonitrile
J_{13} = 3.83463 × (Fraction Gauche) + 4.13607
J_{14} = -9.88335 × (Fraction Gauche) + 13.4036

Lambda Constants for the Dimethylazinoyl Group (Ref.2 in full paper)

The experimental couplings were used in combination with estimated H-H couplings for the individual conformers obtained from the Altona procedure,[1] with the aid of empirical electronegativities (γ) of the functional groups, assuming the dihedral angles to be $\phi_{gauche} = 60°$ or $\phi_{trans} = 180°$ between the substituents, or with other chosen values of ϕ_{gauche} and/or ϕ_{trans}. Simple algebra with the average experimental J_{13} and J_{14} and the estimated couplings for the individual conformers produces two independent values of the trans and gauche conformational preferences, which may give nearly the same or fairly often more or less different values, one of which can usually disregarded by inspection.

An average γ value of 0.91 ± 0.05 for the neutral and protonated dimethylamine oxide group was derived as specified by Altona and coworkers.[1,2] from the essentially constant vicinal ethyl proton coupling of 7.28 ± 0.03 Hz of *N*,*N*-dimethylethylamino-*N*-oxide in D_2O over pH values ranging from 2.8-9.65. The observed range of uncertainty of γ is known[8] to not cause significant, if any real difference, in calculations of preferences within experimental error, so the average γ was used to estimate couplings for the individual conformers. It seems surprising that γ changes so little in water over the given pH range, because it means that both the neutral and protonated forms of the oxide groups have the same γ whereas, in contrast, the same general kind of pH changes for amine and carboxyl groups produce significant changes in γ. The γ values obtained by the same procedure for methanol (0.71), ethanol (0.8), isopropyl alcohol (1.05) and *tert*-butyl alcohol (1.28) show much more variation, however, the value of the percentage of gauche obtained using a γ value for the respective alcohols and a γ value of 0.91 (similar to water) did not show a much variation, if at all in the range of experimental error ($\pm$ 3%).

1. Altona, C.; Ippel, J. H.; Westra, H.; Aldert, J. A.; Erkelens, C.; Groesbeek, M.; Donders, L. A.; *Magn. Reson. Chem.* **1989**, *27*, 564-576.; Altona, C.; Francke, R.; de Haan, R.; Ippel, J. H.; Daalmans, G. J.; Hoekzema, A. J. A. W.; van Wijk, J. *Magn. Reson. Chem.* **1994**, *32*, 670-678.